Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 5.60e-11 cm3/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.07e-01

Confidence level: 7.62e-01

Nearest Neighbors from the Training Set

Image not found

2-Methyl-p-benzoquinone
Measured: 2.35e-11
Predicted: 2.15e-11